Neural Networks and Deep Learning 2

-Statistical Learning and Data Mining-

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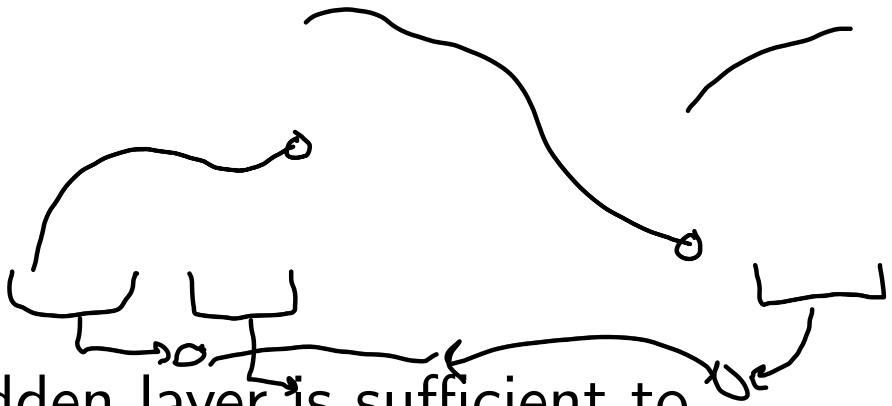
Neural networks: General form

Generalizing to multi-layer neural networks, we can specify any number of hidden units:

(I'm eliminating the bias term for simplicity)

$$\begin{aligned}
\text{0 Layer} &:= \sigma(\alpha_{\text{lowest}}^{\top} X) \\
\text{1 Layer:} &= \sigma(\alpha_{\text{lowest}+1}^{\top}(\text{0 Layer})) \\
&\vdots \\
\text{Top Layer} &:= \sigma(\alpha_{\text{Top}}^{\top}(\text{Top - 1 Layer})) \\
L(\mu_g(X)) &= \beta_{g0} + \beta_g^{\top}(\text{Top Layer}) \quad (g=1,\ldots G)
\end{aligned}$$

Neural networks: General form



Some comments on adding layers:

- It has been shown that one hidden layer is sufficient to approximate any piecewise continuous function

  (However, this may take a huge number of hidden units (i.e. $K >> 1$))

- By including multiple layers, we can have fewer hidden units per layer. Also, we can encode (in)dependencies that can speed computations

Returning to Doppler function

Neural networks: Example

We can try to fit it with a single layer NN with different levels of hidden units K

A notable difference with B-splines is that 'wiggliness' doesn't necessarily increase with K due to regularization

Some specifics:

- I used the R package neuralnet

  (This uses the resilient backpropagation version of the gradient descent)
- I regularized via a stopping criterion ($||\partial\ell||_\infty < 0.01$)
- I did 3 replications

  (This means I did three starting values and then averaged the results)
- The layers and hidden units are specified like

  3 4 5

  (# Hidden Units on Layer 1) (# Hidden Units on Layer 2)...

Neural networks: Example

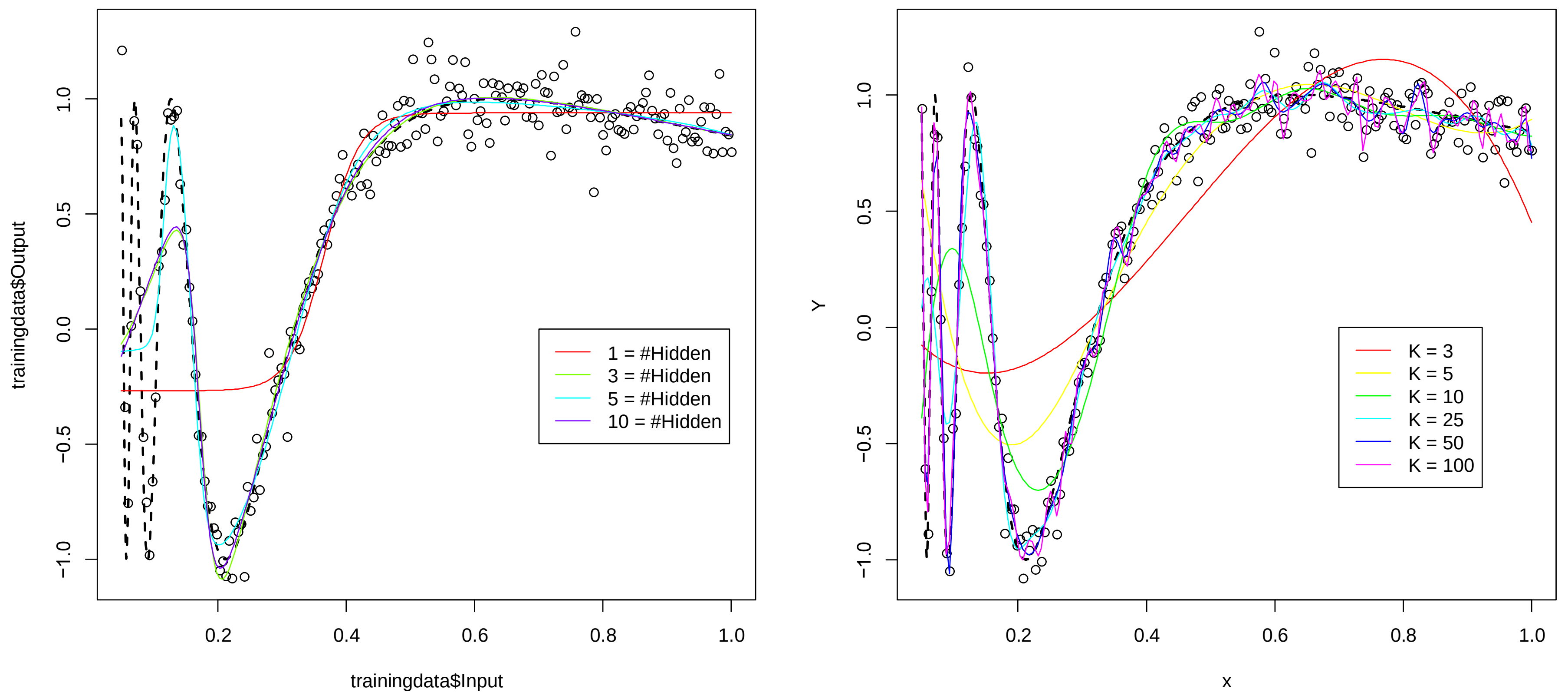


Figure: Single layer NN vs. B-splines

Neural networks: Risk

What's the estimation equality? $IMSE = \int \mathbb{E}(\hat{f}(X) - f_*(X))^2 \, d\mathbb{P}_X$

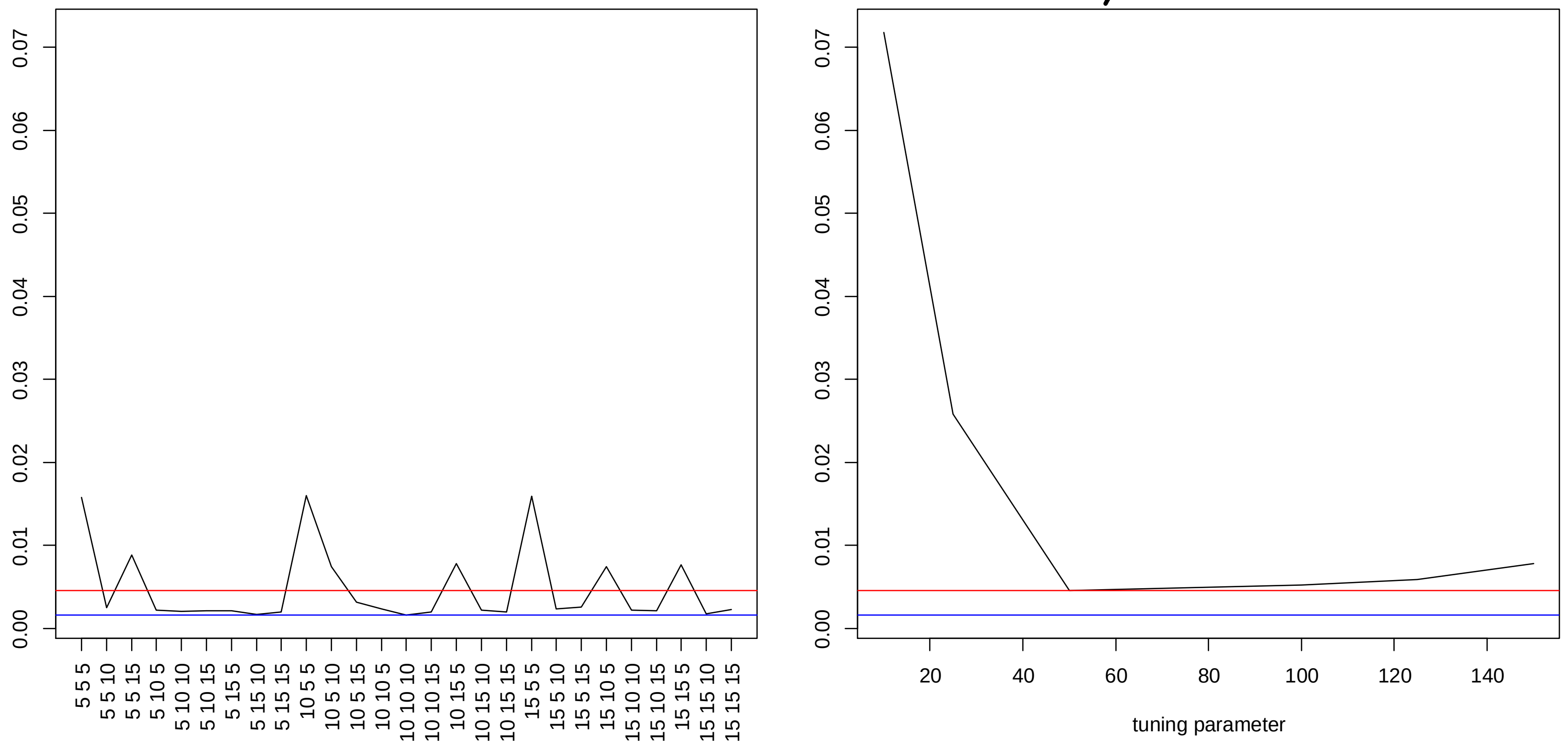


Figure: 3 layer NN[1] vs. B-splines

[1]The numbers mean (#(layer 1) #(layer 2) #(layer 3))

Neural networks: Example

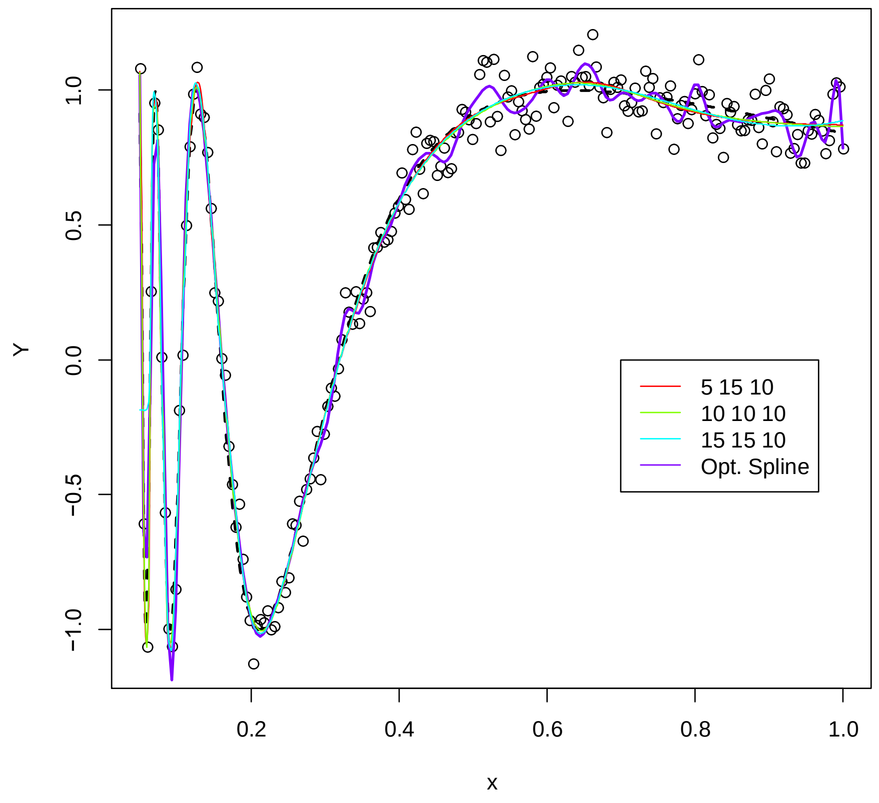


Figure: Optimal NNs vs. Optimal B-spline fit

Neural networks: Code for Example

```
trainingdata  = cbind(x,Y)
colnames(trainingdata) = c("Input","Output")
testdata      = xTest

require("neuralnet")
K          = c(10,5,15)
nRep       = 3
nn.out     = neuralnet(Output~Input,trainingdata,
                       hidden=K, threshold=0.01,
                       rep=nRep)
nn.results = matrix(0,nrow=length(testdata),ncol=nRep)
for(reps in 1:nRep){
  pred.obj = compute(nn.out, testdata,rep=reps)
  nn.results[,reps] = pred.obj$net.result
}
Yhat = apply(nn.results,1,mean)
```

Hierarchical view

Hierarchical view

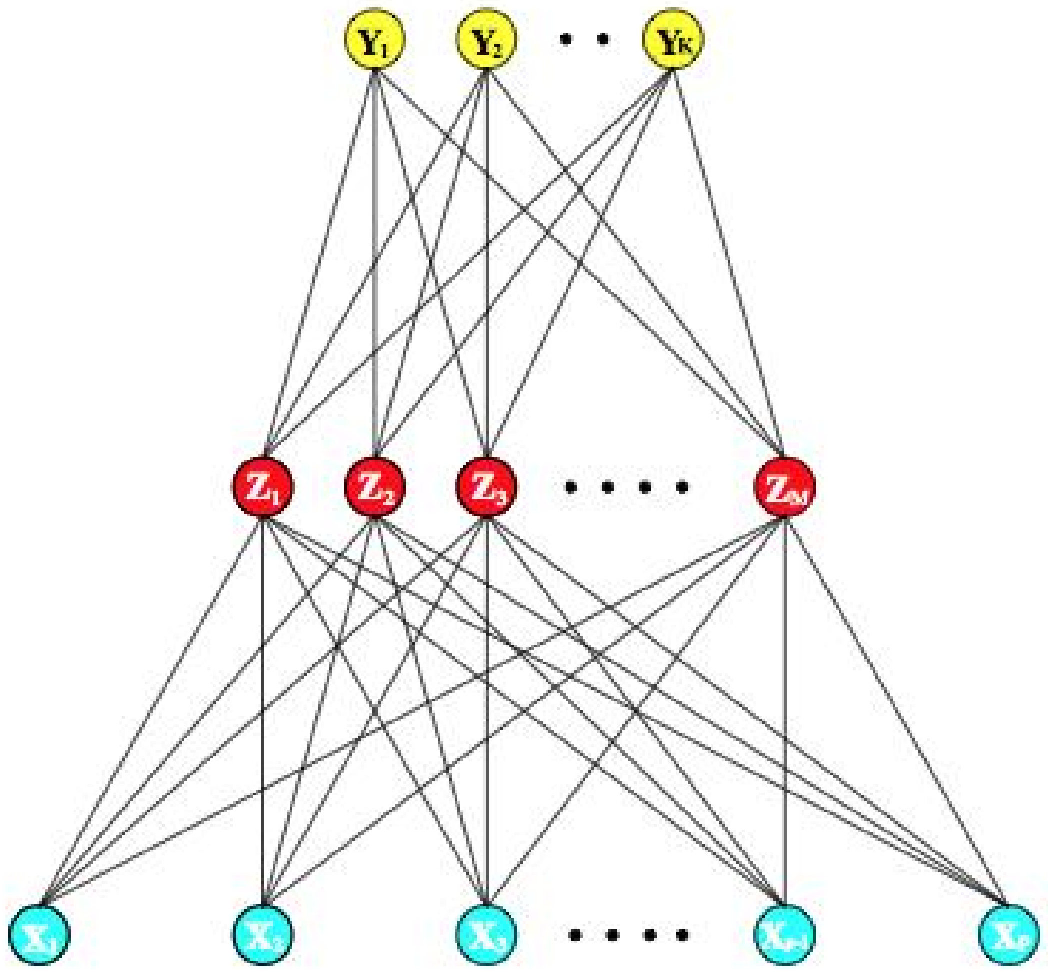


Figure: Recall: Single hidden layer neural network. Note the similarity to latent factor models

Hierarchical from example

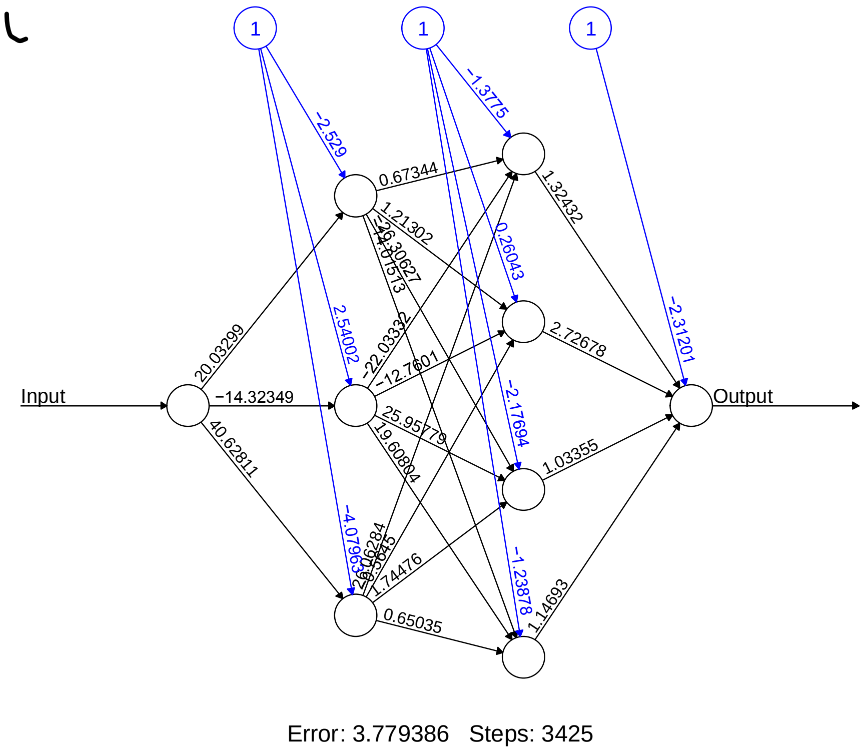
"GRAPHICAL MODEL"

$G = (V, E)$

$$\begin{tikzcd} 1 \arrow[r] & 2 \end{tikzcd}$$

$V = \{1, 2\}$

$E = \{\{1, 2\}\}$



This is a directed acyclic graph (DAG)

```
nn.out = neuralnet(Output~Input,trainingdata,
                              hidden=c(3,4))

plot(nn.out)
```

Neural networks: Localization

One of the main curses/benefits of neural networks is the ability to localize

This makes neural networks very customizable, but commits the data analyst to intensively examining the data

Suppose we are using 1 input and we want to restrict the implicit DAG

Neural networks: Localization

That is, we might want to constrain some of the weights to 0

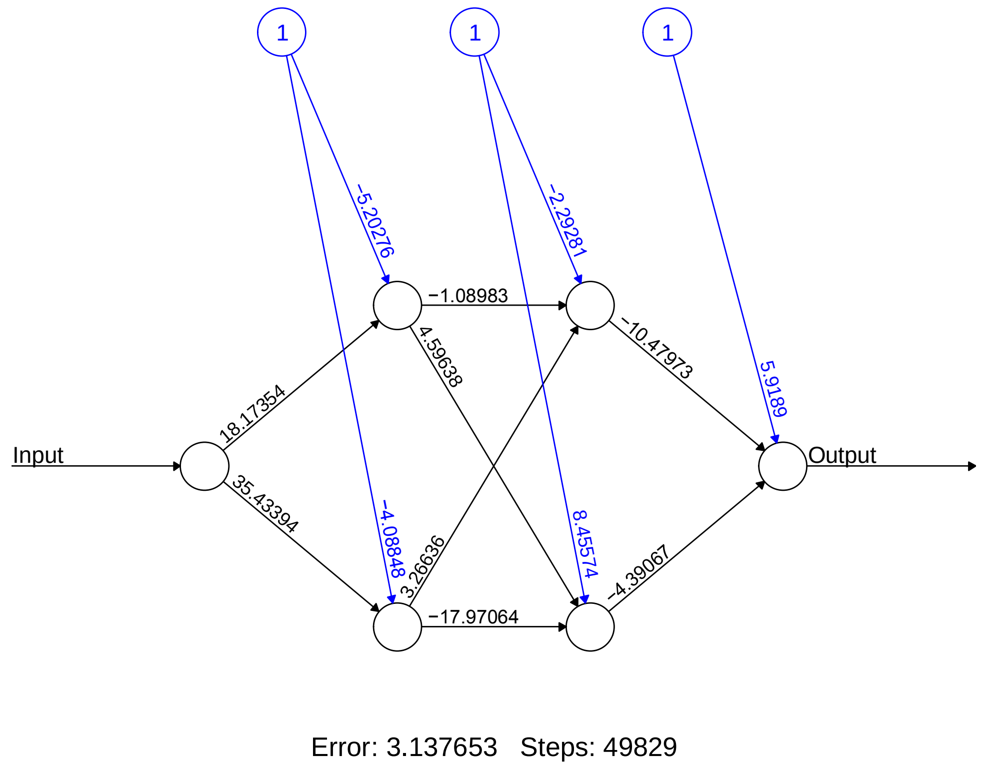


Figure: Unconstrained neural network

```
nn.out = neuralnet(Output~Input,trainingdata,
                   hidden=c(2,2))
```

Neural networks: Localization

We can do this in neuralnet via the exclude parameter

To use it, do the following:

```
exclude = matrix(1,nrow=2,ncol=3)
exclude[1,] = c(2,2,2)
exclude[2,] = c(2,3,1)
nn.out = neuralnet(Output~Input,trainingdata,
                   hidden=c(2,2), threshold=0.01,
                   exclude=exclude)
```

exclude is a $E \times 3$ matrix, with E the number of exclusions

- first column stands for the layer
- the second column for the input neuron
- the third column for the output neuron

Neural networks: Localization

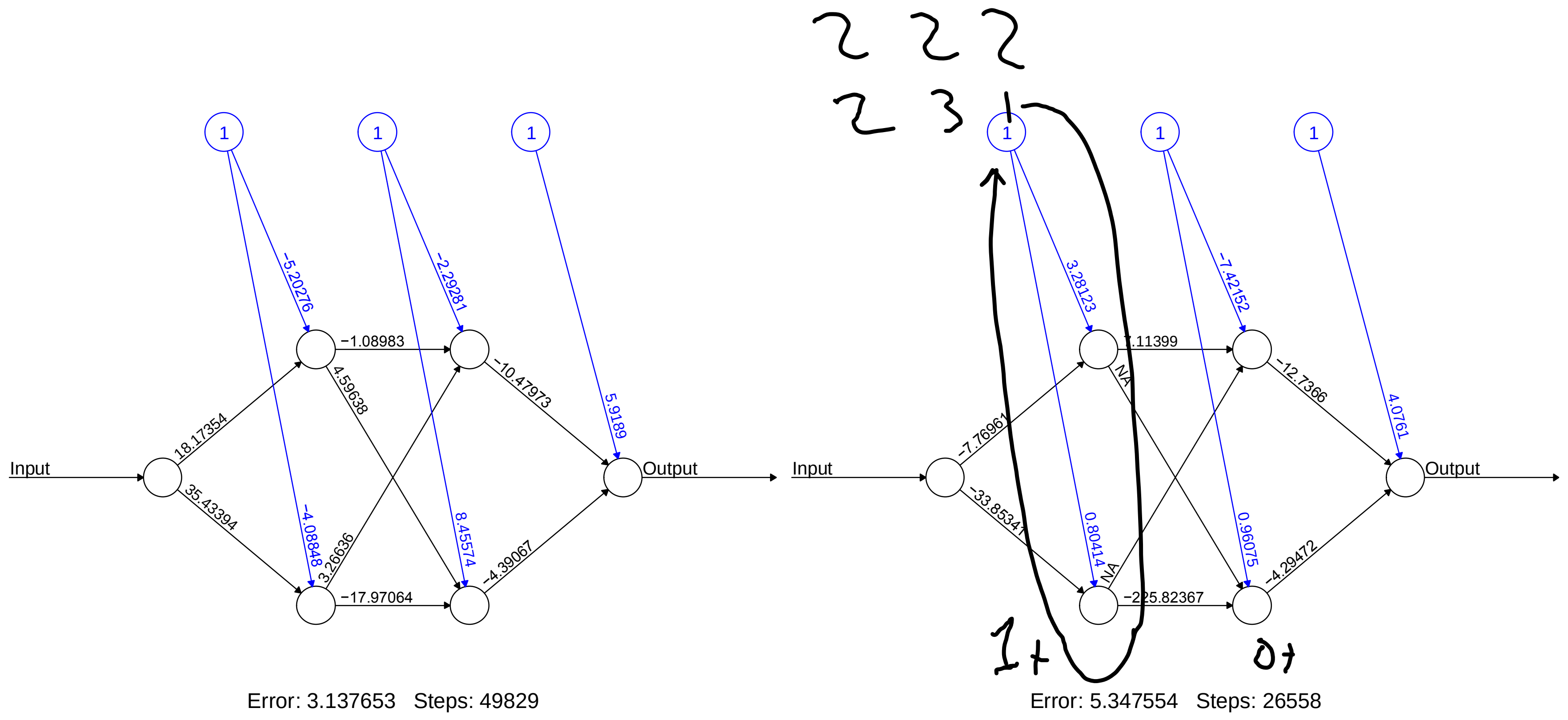
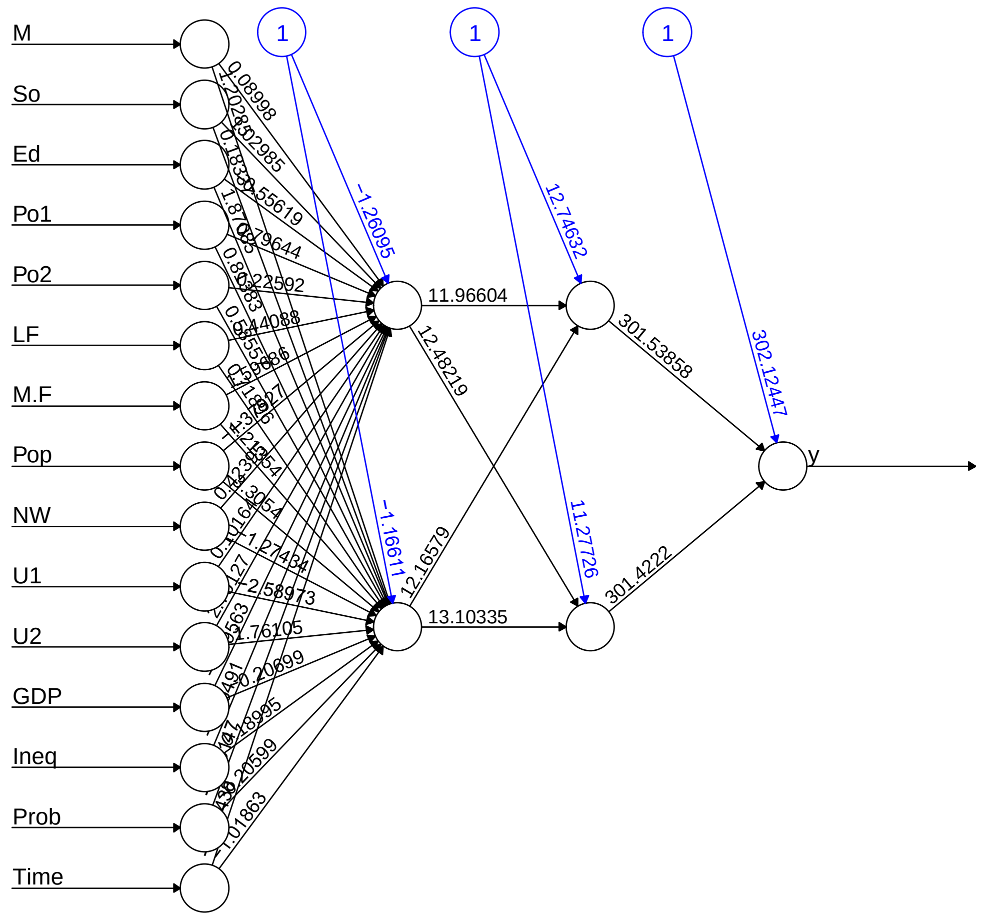


Figure: Not-constrained vs. constrained

Neural networks: Crime data

```
M
percentage of males aged 14–24.
So
indicator variable for a Southern state.
Ed
mean years of schooling.
Po1
police expenditure in 1960.
LF
labour force participation rate.
M.F
number of males per 1000 females.
...
y
rate of crimes in a particular category per capita
```

Neural networks: Crime data



Neural networks: Crime data

We may want to constrain the neural network to have neurons specifically about

- Demographic variables
- Police expenditure
- Economics

This type of prior information can be encoded via exclude

(This is, in my opinion, when neural networks work well)

Tuning parameters

Neural networks: Tuning parameters

The most common recommendation I've seen is to take the 3 tuning parameters: The number of hidden units, the number of layers, and the regularization parameter λ

(or a stopping criterion λ for the iterative solver)

Either choose $\lambda = 0$ and use risk estimation to choose the number of hidden units

(This could be quite computationally intensive as we would need a reasonable 2-d grid over units $\times$ layers)

Or, fix a large number of layers and hidden units and choose λ via risk estimation

(This is the preferred method)

Neural networks: Tuning parameters

We can use a GIC method:

$$\text{AIC} = \text{training error} + 2\hat{df}\,\hat{\sigma}^2$$

(This is reported by neuralnet, by setting likelihood $=$ T)

Or via cross-validation

Neural networks: Tuning parameters

Unfortunately, neuralnet provides a somewhat bogus measure of AIC/BIC

Here is the relevant part of the code

```
if (likelihood) {
  synapse.count = length(weights) - length(exclude)
  aic = 2 * error + (2 * synapse.count)
  bic = 2 * error + log(nrow(response))*synapse.count
}
```

They use the number of parameters for the degrees of freedom!